TRIM.FaTE USER'S GUIDE MODULE 8: LINKS AND ALGORITHMS¹

Transport of chemical mass between compartments and transformation between different chemicals within a compartment in a TRIM.FaTE scenario is facilitated through the use of links and algorithms. Links (described in Section 1) determine the pathways for mass transport or transformation/degradation in the system, with each link referencing one or more algorithms (described in Section 2) that mathematically represent the mass transfer or transformation/degradation. Links are always between compartments (including sinks), and never between volume elements or other TRIM.FaTE objects. This module provides information on creating, removing, and configuring links and algorithms in TRIM.FaTE.

1. LINKS

After importing the spatial layout and selecting the compartments for each volume element, the next step in setting up a TRIM.FaTE simulation is specifying the links between compartments. A link is a TRIM.FaTE object defined as a "connection" that allows the transfer of chemical mass between compartments, the degradation of a chemical present in a compartment (where the mass is then transferred to a degradation sink), or the transformation of one modeled chemical to another modeled chemical. Links can exist between any two compartments with one or more algorithms describing chemical transport between them, or from a compartment to itself if transformation of chemical mass is being modeled. Links are always **unidirectional**; however, it is not unusual for two links to exist between two compartments (i.e., one to and one from each compartment). Typically, links are created between the following general types of compartments:

- Between adjacent abiotic media;
- Between abiotic media and advection or flush rate sinks;
- Between biotic compartments and abiotic media;
- Between biotic compartments;
- Between compartments and degradation sinks; and
- Within compartments where chemicals are transformed.

Although this is not intended to be an exhaustive list of possible types of links, it does provide an idea of types of relationships links are designed to describe. For more information on how links are implemented within the TRIM.FaTE conceptual framework, refer to Chapter 5 of Volume I of the Technical Support Document for TRIM.FaTE (U.S. EPA 2002).

The remainder of this section addresses the following topics.

- How are links created? (Section 1.1)
- Why and how are links selected? (Section 1.2)

¹Descriptions of library-specific algorithms and properties presented in this module pertain to the March 2003 versions of the TRIM.FaTE library.

- What are link properties? (Section 1.3)
- Why and how are links removed? (Section 1.4)

1.1 How Are Links Created?

Links can be created in three different ways:

- Manually (Section 1.1.1);
- Using Smart Link (Section 1.1.2); and
- Using a Property Import file (Section 1.1.3).

These three methods can be used individually or in combination to create all of the links for a scenario. Based on experience to date, the most efficient and least error-prone approach has proven to be the use of both the Smart Link tool and a Property Import file. This combined approach is described in Section 1.1.4.

1.1.1 Creating Links Manually

Creating links manually is the most straightforward method for creating links, as it only involves selecting two (or more) compartments and clicking the "<<Link>>" button. Users may find this method convenient for simple scenarios. However, for more complex scenarios, this method can be quite time consuming and prone to user error.

To create links manually, the user should follow these steps.

- (1) Select the Links view in the Scenario Window. There will be two identical "Outdoor Environment" columns on the left side of the tab. (See Figure 1)
- (2) Select the "Compartments" option from the drop-down menu at the top of each column. (See Figure 1)
- (3) Select the compartment(s) in the left and right columns that will be linked together. Note that more than one compartment can be selected from one of the columns (i.e., in order to create multiple links simultaneously), but multiple compartments cannot be selected from *both* columns.
- (4) To link the compartments, click the "<<Link>>" button at the bottom of the right column

When two compartments are linked manually, both possible links (i.e., both to and from both linked compartments) are created automatically; in other words, a "one-way" link between two compartments cannot be created manually. It should be noted that in order to model chemical transformation, compartments must be linked to themselves. To add these links, the user should select the same compartment in the left and right columns in Step 3.

When manually adding links, TRIM.FaTE places no restrictions on where links can be formed. For example, if the user asks the model to place a link between air and sediment, the model will create the link, even though there may be no algorithms in the library to transport mass between these compartments. The model will not use the link, however, unless there are algorithms that describe transport or transformation between the linked compartments. The primary drawback of adding unused links is that they complicate the setup unnecessarily and may make it more difficult to diagnose sources of problems in a scenario.

1.1.2 Creating Links Using Smart Link

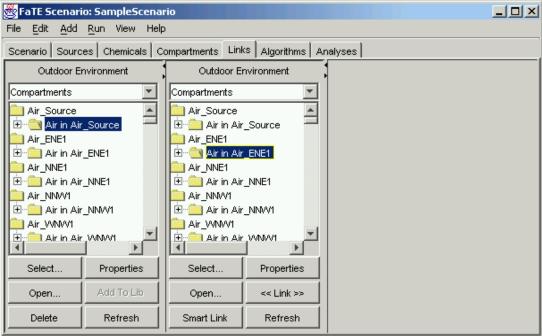
To create links using Smart Link, the user would select volume elements and click "Smart Link," and the model will create links for the compartments in the selected volume elements for which the enabled algorithms in the library apply and which meet certain criteria. With regard to these criteria, TRIM.FaTE first identifies the algorithms in the TRIM.FaTE library that apply to the chemicals selected for the scenario. Smart Link then creates links between each pair of compartments in the selected volume elements whose *Category* properties match the *sendingCompartmentCategory* and *receivingCompartmentCategory* properties of any of the identified algorithms, provided the pair of compartments has an appropriate relationship for the algorithm. This relationship is determined in one of two ways. For algorithms which specify a value for the *compartmentRelationship* property, only the relationship defined by the value of this property is considered appropriate. For algorithms without a *compartmentRelationship* property, the following relationships are considered appropriate:

- compartments in adjacent volume elements;
- compartments co-located within a volume element; and
- within any compartments where transformation between different chemicals is possible.

Even if multiple algorithms are available to transport mass between a given pair of compartments or transform mass within a compartment, only one link will be created by Smart Link (i.e., multiple algorithms can exist on a single link).

²For more detailed descriptions of these compartment and algorithm properties, refer to Module 4, Adding New Components to a Library.

Figure 1 Creating Links Manually



The Smart Link process creates links between abiotic and biotic compartments and any sinks defined for the scenario. Users should note that flush rate sinks and degradation sinks must be manually added to the scenario prior to performing Smart Link to allow the links to be created between the compartments and sinks. Advection sinks are automatically added to appropriate volume elements (i.e., volume elements with at least one side comprising a boundary of the modeled region) when Smart Link is performed.

This method, unlike the manual method, will not create any links that do not have associated algorithms. The

IMPORTANT POINTS ABOUT SMART LINK

- If the compartment relationship for an algorithm allows links to be created between compartments within a volume element and between compartments in adjacent volume elements, Smart Link will only create the link between the compartments located within the same volume element. Smart Link create links between eligible compartments in adjacent volume elements only if a link cannot be created between compartments within a single volume element.
- Smart Link does not create links to degradation and flush rate sinks. These links will need to be created by the user (either manually or via a Property Import file).

compartments that are linked by Smart Link are only those that are able to exchange mass based on the available TRIM.FaTE algorithms; the reverse link between a pair of compartments is not created. For example, if an eagle and a shrew are located in the same volume element, and an algorithm exists for consumption of shrews by eagles, a link will be created from the shrew to the eagle but *not* vice-versa; that is, the *reverse* link from eagle to shrew will not be created.

To create links using Smart Link, the user should follow these steps.

- (1) Select the Links view in the Scenario Window. There will be two identical "Outdoor Environment" columns on the left side of this view. (See Figure 2)
- (2) Select the "Volume Elements" option from the drop-down menu at the top of each column. (See Figure 2)
- (3) Select from the left or right column the volume element(s) with which the compartments to be Smart Linked are associated. It is necessary to select the volume element(s) in only *one* of the two columns; the second column is not used when creating links using Smart Link. (See Figure 2)
- (4) To Smart Link the compartments in the selected volume elements, select the "Smart Link" button at the bottom of the right column. (See Figure 2)



Figure 2
Creating Links Using Smart Link

The biggest advantage of the Smart Link feature, other than the time savings over manually specifying all links, is that it allows the user to let the model determine the appropriate links between the compartments in the selected volume elements and prevents the omission of necessary links due to user oversight. However, **Smart Link cannot be relied upon to create all of the necessary links in every situation.**

In particular, there are two types of situations where Smart Link fails to create all of the necessary links.

• When there are multiple adjacent volume elements with compartments of a given type that could be linked³ with a biotic compartment in a particular volume element. In this case, the model cannot select which compartment in the adjacent volume elements to link to the biotic compartment, and thus it does not create a link. For example, a surface soil volume element with a raccoon compartment may be adjacent to two different surface water volume elements containing fish compartments that comprise the raccoon's diet (i.e., algorithms exist to allow the raccoon to receive mass from the fish compartments via ingestion). Because the model does not know from which of these surface water volume elements the raccoons typically feed (or whether the raccoon should feed from both surface water bodies), it does not create a link via Smart Link. In situations such as this, Smart Link will give a "Multiple Compartments Match" warning, and the user must add the link manually. For this example, TRIM.FaTE would provide the following warning:

Multiple Compartments Match: For algorithm Ingestion of Water Column Herbivore by Raccoon(AlgInstID_2605), multiple compartments can be linked to receiving compartment Raccoon in SurfSoil SW2 so algorithm could not be smart linked.

When there is a need to link biotic compartments associated with one volume element to a compartment(s) in a non-adjacent volume element. In this case, the model considers an algorithm during the Smart Link process but cannot find "possible" compartments to be linked because the eligible compartments are not in adjacent volume elements. For example, there may be an ingestion algorithm allowing transfer of mass from a benthic fish compartment (associated with a sediment volume element) to a raccoon compartment (associated with a surface soil volume element). Surface soil volume elements would not be adjacent to sediment volume elements if these volume elements have no shared surfaces (i.e., they would not be adjacent because their vertical dimensions place these volume elements at different heights, even if the surface soil volume element is horizontally adjacent to a sediment compartment). Therefore, Smart Link will not create any links for this ingestion algorithm. In situations like this, Smart Link will give a "No Compartments Match" warning specifying the algorithm and the compartments that could not be linked. For this example, TRIM.FaTE would provide the following warning:

No Compartments Match: For algorithm Ingestion of Benthic Omnivore by Raccoon, no compartments can be linked to compartment Raccoon in SurfSoil_E1 so algorithm could not be smart linked.

³ Possible links are those for which there are algorithms in the library that can transport mass between these compartments and the particular biotic compartments.

For both of these situations, the user may need to supplement the links created by Smart Link with links created manually and/or with a Property Import file. To determine the additional necessary links following the use of the Smart Link feature, the user should review the list of warnings created by Smart Link. For each warning labeled as "No Compartments Match" or "Multiple Compartments Match," the user needs to decide whether an additional link is necessary.

In addition, it is possible that the Smart Link process could create links that are not desired for a scenario due to particular site-specific conditions. For example, a user may wish to set up the food chain to "force" certain types of biota to obtain their food (e.g., prey compartments) from a volume element not adjacent to the one containing that biotic compartment, even if the food compartment is also present in the same volume element. The user would need to manually delete or disable the link between the predator and prey compartments in the same volume element. These situations will depend on site-specific characteristics, and it is up to the user to ensure that the links required for their planned scenario are created.

It is important to note that it is not unusual for the model to generate many warnings during the Smart Link process. Many of these warnings simply confirm that the scenario is configured properly. For example, the current TRIM.FaTE library contains an algorithm for the ingestion of worms by raccoons. Given this, if a worm compartment is included in one volume element of a scenario using this library, but there are no raccoon compartments in the same or adjacent volume elements, the user will receive a "No Compartments Match" warning indicating that there are no raccoon compartments to link with the worm compartment for the implementation of this algorithm. If the user does not want this worm compartment to be consumed by raccoons, this warning will not be a concern for this particular scenario. However, there are usually several warnings in each scenario that do require the user to add additional links. As a result, it is strongly recommended that the user review the list of warnings thoroughly before proceeding with configuring a scenario.

Note that following the Smart Link process, the user may want to modify the system of links for a scenario to better represent the spatial aspects of the food chain for certain animals at that site. For example, the user could implement links to compartments in some non-adjacent volume elements so that the diet can be fractionated spatially. Refer to Module 12 for additional information on setting up the food chain for a scenario.

1.1.3 Creating Links Using a Property Import File

Creating links using a Property Import file is similar to creating links manually in that it involves specifying each link to be created individually. However, unlike creating links manually, the setup for this method only needs to be configured one time for each scenario and then can be reused for multiple scenarios.

To create links using a Property Import file, the user should follow these steps.

(1) Create a Property Import file containing the links to be created (guidance on how to create a Property Import file and the format required for this file is included in

- Module 3). Note that, if desired, these links can be included in the same Property Import file that may be used to set compartment and scenario properties. (See Figure 3)
- (2) Select the "Load Properties from a File" from the "File" menu in a Scenario Window. (See Figure 4)
- (3) Click the "Browse" button in the Load Properties window. Use the file browser to find the Property Import file created in Step (1). Select the file and click the "Open" button. (See Figure 4)
- (4) Select the run name under "Runs" and click the "Override" button. If the file is configured correctly, the model will open a window with the message: "The properties were overridden successfully." Click the "OK" button. If the file is not configured correctly, an error window will appear detailing the problem with the Property Import file. (See Figure 4)

Figure 3. Example of Property Import File

```
Version: 1
Scenario: FullMaine
Run: BaseRun
Scenario: FullMaine
    SendingCompartment: Bald Eagle in SurfSoil_E1
  ReceivingCompartment: Surface water in SW_Penob
        ReciprocalLink: Surface water in SW_Penob to Bald Eagle in SurfSoil_E1
             Algorithm: Default
NewLink:
    SendingCompartment: Black-capped Chickadee in SurfSoil_E1
 ReceivingCompartment: Surface water in SW_Penob
        ReciprocalLink: Surface water in SW_Penob to Black-capped Chickadee in
SurfSoil_E1
             Algorithm: Default
NewLink:
    SendingCompartment: Long-tailed Weasel in SurfSoil_E1
  ReceivingCompartment: Surface water in SW_Penob
      ReciprocalLink: Surface water in SW_Penob to Long-tailed Weasel in SurfSoil_E1
             Algorithm: Default
NewLink:
    SendingCompartment: Mink in SurfSoil_E1
  ReceivingCompartment: Surface water in SW_Penob
        ReciprocalLink: Surface water in SW_Penob to Mink in SurfSoil_E1
             Algorithm: Default
```

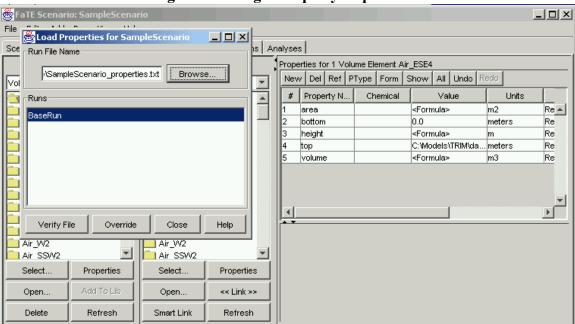


Figure 4. Using a Property Import File

Like the manual method, creating links using a Property Import file places no restrictions on where links can be formed, thus allowing the user to create links with no associated algorithms. The primary drawback of adding unused links is that they complicate the setup unnecessarily and may make it more difficult to track down problems following a run.

1.1.4 Using Smart Link in Combination with a Property Import File

A Property Import file can used in combination with Smart Link to efficiently create all of the links required for a scenario while minimizing potential user error.

To combine the use of Smart Link and the Property Import file, the user should follow these steps.

- (1) Perform a Smart Link for all volume elements in a scenario.
- (2) Examine the warnings to determine which necessary links were not created by Smart Link.
- (3) Compile a Property Import file to create each of these links (or disable any undesired links).
- (4) Import the Property Import file as described in Section 1.1.3. After completing this step, all of the necessary links for the scenario will have been created.

1.2 Why and How Are Links Selected?

To access link properties (described in Section 1.3) or remove links (described in Section 1.4), the links must be selected. Links existing within a scenario can be selected using the TRIM.FaTE graphical user interface (GUI) in two ways:

- Manually (Section 1.2.1); and
- Using the Select Tool (Section 1.2.2).

1.2.1 Manual Selection of Links

Links associated with a particular volume element and/or compartment can be selected manually. It is particularly useful when the user would like to select a limited number of links for a particular compartment.

To select links manually, the user should follow these steps.

- (1) From the Scenario window, select the Compartments, Links, or Algorithms Tab. (See Figure 5)
- (2) Select the "Volume Elements," "Compartments," or "Links" option from the drop-down menu at the top of one of the Outdoor Environment panes. Note that only one Outdoor Environment pane is used to select links; the second Outdoor Environment pane can be ignored. If "Volume Elements" is selected, proceed to step (3). If "Compartment" is selected, skip to step (4). If "Links" is selected, skip to step (5). (See Figure 5)
- Ouble-click the volume element of interest in the Outdoor Environment pane to reveal the compartments associated with the volume element. (See Figure 5)
- (4) Select the compartment of interest in the Outdoor Environment pane and reveal the links associated with the compartment by either double-clicking on the compartment or clicking the "+" symbol in front of the compartment name. (See Figure 6)
- (5) Scroll through the list of links in the Outdoor Environment pane and select the link (or links) of interest by clicking on the name of the link(s). (See Figure 7)

After selecting one or more links, the user will be able to view and edit the properties of that link using the Property Editor window that appears (see Section 1.3).

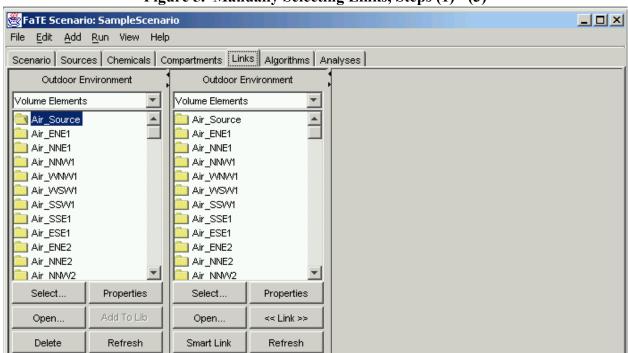
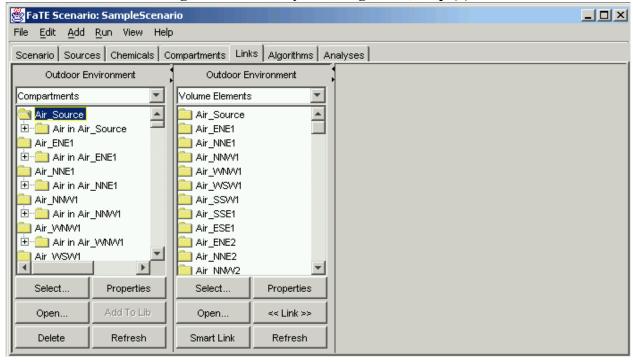


Figure 5. Manually Selecting Links, Steps (1) - (3)





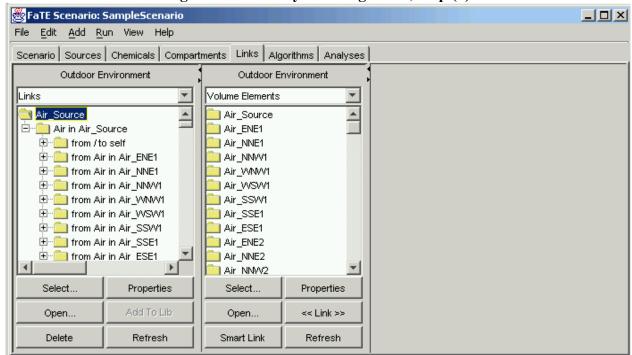


Figure 7. Manually Selecting Links, Step (5)

1.2.2 Using the Select Tool

The Select Tool can be used to select groups of related links with a minimal amount of user interaction. This tool is particularly useful when the user would like to review or edit the properties of related links, or delete a group of related links.

To select links using the Select Tool, the user should follow these steps.

- (1) From the Scenario window, select the Compartments, Links, or Algorithms Tab. (See Figure 8)
- (2) Select the "Links" option from the drop-down menu at the top of one of the Outdoor Environment panes. (See Figure 8)
- (3) Click the "Select..." button below the Outdoor Environment Tab. (See Figure 8)
- (4) Fill in the necessary information in the "Select..." window. Select "Link" from the "Type is:" drop-down menu. (See Figure 9)
- (5) Click the "Select" button at the bottom left of the "Select..." window. A window will appear to indicate the number of links that were selected. (See Figure 10)

After clicking "OK" in this window, the properties for the selected links will appear in the Property Editor window on the right side of the Scenario Window. The user will now be able to edit these properties if desired (see Section 1.3).

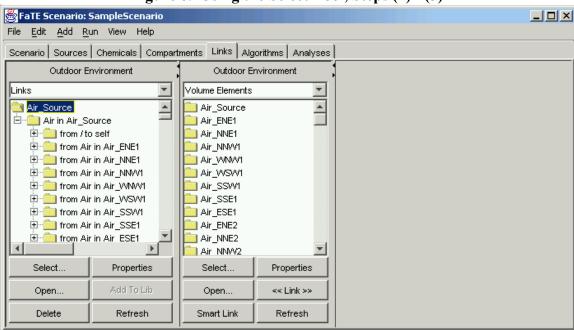
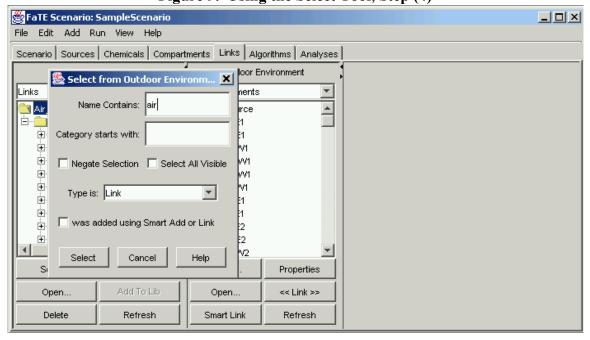


Figure 8. Using the Select Tool, Steps (1) - (3)





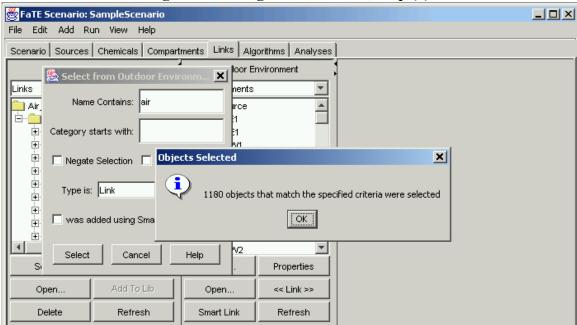


Figure 10. Using the Select Tool, Step (5)

1.3 What Are Link Properties?

Links, like compartments and volume elements, have properties associated with them. Some link properties are included for all links (e.g., enabled) while others are only associated with particular types of links. For example, the link property <code>BulkWaterFlowRate_Volumetric</code> is only included on links between connected surface water compartments (e.g., two adjacent river compartments) and is used to specify the flow between the two compartments. Typically, the user will not be required to manually add these link properties to the scenario as they are automatically added as needed during the "Verify" process or may be added by the user in a Property Import file (see Module 3) when setting up a scenario. However, the user may be required to provide values for some link properties in a scenario.

The values for link properties can be set using the Property Editor on the Compartments, Links, or Algorithms Tab or using a Property Import file (described in Module 3). Users may find it convenient and easier to assure quality to set all link properties using a Property Import file. It is important to note that link properties cannot be set until the links are created, and thus users cannot set link properties in the same Property Import file used to create links (see Section 1.1.3).

To access link properties, the user should follow these steps.

(1) Select the link from the Outdoor Environment pane (using one of the methods described in Section 1.2). (See Figure 11)

(2) Click the "Properties" button under the Outdoor Environment pane. (See Figure 11)

A link property will typically provide information related to mass flows between two compartments. The specific link properties required for a scenario will depend on the individual compartments and algorithms included in the scenario. Some link properties applied in TRIM.FaTE test scenarios to date include the following:

- Fraction of total erosion and total runoff that is applied between surface soil compartments and adjacent surface soil and/or surface water compartments (see Module 11);
- Properties related to water flowing from one surface water compartment to another (e.g., distance between midpoints of the water bodies; diffusive exchange coefficient of the water; volumetric flow of water);
- Water flow from groundwater compartment to a surface water compartment; and
- Diet fraction properties to account for animals feeding on a given food type from multiple locations (e.g., a hawk feeding on mice located in two or more volume elements; refer to Module 6).

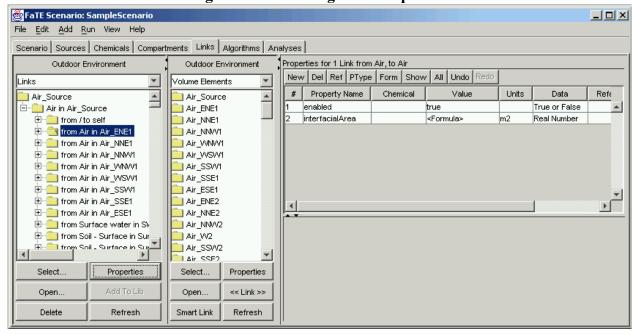


Figure 11. Accessing Link Properties

In addition, the property *enabled* is applied to all links by default with a value of "true." The user can reset this property to "false" to disable a link (i.e., to eliminate mass transfer or transformation via that path; see Section 1.4).

Users can add new properties to links using the Property Editor or a Property Import file, provided the property types associated with the new properties are included in the library referenced by the scenario. These additional properties may be useful if existing link properties are set to formulas and intermediate calculations are desired. The user is reminded that the Property Editor will only add properties to those links selected in the Links view of the Scenario Window when the Property Editor is opened (by clicking the "Properties" button). Accordingly, this approach may have greater potential for oversights, making the use of a Property Import file the preferable approach in many situations.

1.4 Why and How Are Links Removed?

A user may wish to remove a link from a scenario in order to either adapt a scenario to a site-specific conceptual framework (e.g., to create a desired food web) or for testing/diagnostic purposes. If the user may wish to reinstate the link at a later time (e.g., after testing), it is recommended that the link be disabled rather than removed.

To remove a link from a scenario, the user should follow these steps.

- (1) Select the link (or links) from the Outdoor Environment pane (using one of the methods described in Section 1.2).
- (2) Click the "Delete" button under the Outdoor Environment pane.

To disable a link without deleting it from a scenario, the user should follow these steps.

- (1) Select the link (or links) from the Outdoor Environment pane (using one of the methods described in Section 1.2).
- (2) Click the "Properties" button under the Outdoor Environment pane.
- Change the value of the *enabled* property to "false" in the Property Editor. When enabled is set to "false," the model will ignore the link and any associated link properties and algorithms. The value can be changed back to "true" later if desired. Note that setting *enabled* to "false" will disable only the selected link; other links between the same types of compartments will not be affected.

2. ALGORITHMS

Algorithms are TRIM.FaTE objects that mathematically represent the mass transfer between two linked compartments or transformation of mass within a compartment. One or more algorithms can be associated with a given link, with each algorithm designed to represent the mass transfers associated with a particular process (e.g., advection, diffusion). The remainder of this section addresses the following topics:

- What are algorithm properties? (Section 2.1)
- How are algorithms added to links? (Section 2.2)
- Why and how are algorithms removed from a link (Section 2.3)

2.1 What Are Algorithm Properties?

Algorithms, like links, compartments, and volume elements, have properties associated with them. There are several special algorithm properties that control the compartments and chemicals to which the algorithm will apply and whether the algorithm should be used in the scenario. Table 1 provides a description of each of these properties Any other properties associated with an algorithm provide data used in calculating the algorithm's *transferFactor* property.

To access algorithm properties, the user should follow these steps.

- (1) Select the link (or links) from the Outdoor Environment pane (as described in Section 1.2).
- (2) Click the "Show Algs" button under the Outdoor Environment pane. The algorithms associated with the selected link will be displayed in the "Algorithms in Links" pane. If multiple links are selected, the algorithms associated with each of the links will be displayed together. (See Figure 12)
- (3) Select the algorithm in the "Algorithms in Links" pane. (See Figure 12)
- (4) Click the "Properties" button under the Algorithms in Links pane. (See Figure 12)

It is important to note that — with the exception of the *enabled* property, whose value may be changed to enable or disable a particular algorithm in a scenario — the changing of algorithm property values or addition of new algorithm properties will typically be done in the library. In addition, the user should be aware that changing the value of an algorithm property (including the *enabled* property) on a single link within a scenario will change the value of the property for that algorithm on **all links in the scenario**.

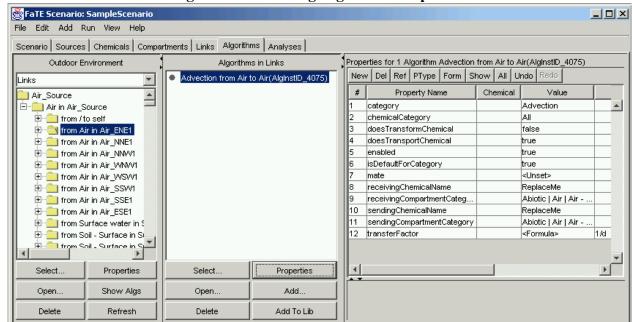


Figure 12. Accessing Algorithm Properties

Table 1. Description of Special Algorithm Properties

Property Name	Data Type	Required	Description
category	category		A hierarchical classification of the process represented by the algorithm (e.g., Ingestion Ingestion of fish by birds)
chemicalCategory	category	T1	The hierarchical classification of chemical to which the algorithm applies (e.g., Mercury Elemental Mercury). The string "All" can be used to denote that the algorithm applies to all modeled chemicals. If not specified, the model assumes "All". This property should be " <unset>" for transformation algorithms.</unset>
compartmentRelationship	string		This property should be used when the sending and receiving compartments have a specific spatial relationship with one another. Allowable values are: • ANY - algorithm applies regardless of relationship between compartments (this is the default for this property) • SAME - algorithm applies within same compartment (i.e., for transformation algorithms) • SENDER_ABOVE - algorithm applies when sender is above receiver • SENDER_BELOW - algorithm applies when sender is below receiver • NEXT_TO - algorithm applies when receiver is horizontally next to sender • IN_SAME_VOLUME_ELEMENT - algorithm applies when receiver and sender are in same volume element but not in same compartment • ABOVE_OR_BELOW - algorithm applies when receiver is above or below sender • ADJACENT - algorithm applies when sender is above, below, or horizontally next to receiver

Property Name	Data Type	Required	Description
doesTransformChemical	boolean	Т	This property indicates whether the algorithm transforms chemicals within a compartment.
doesTransportChemical	boolean	T	This property indicates whether the algorithm transports chemicals between compartments.
enabled	boolean	Т	This property indicates whether the algorithm is enabled in the scenario. The default value is "true."
isDefaultForCategory	boolean	T	If multiple algorithms with the same category apply to a link, this property indicates if this algorithm should be the one used. The default value is "true." This feature is not enabled in Ver 2.7.
mate	string		This property indicates the name of the algorithm that should be used on reciprocal links.
receivingChemicalName	string	T ¹	This property indicates the name of the chemical on the receiving side of the link.
receivingCompartmentCategory	category	T	This property indicates the hierarchical classification of the receiving compartment to which this algorithm applies (e.g., Abiotic Air Air - Default; Mammal Raccoon).
sendingChemicalName	string	T ¹	This property indicates the name of the chemical on the sending side of the link.
sendingCompartmentCategory	category	Т	This property indicates the hierarchical classification of the sending compartment to which this algorithm applies.
transferFactor	floating- point	Т	The transfer factor for the algorithm.

¹ An algorithm must have either (1) the *chemicalCategory* or (2) the *receivingChemicalName* and *sendingChemicalName* defined. If both are defined, the *chemicalCategory* overrides the chemical names. For transformation algorithms, the chemical names **MUST** be used and the *chemicalCategory* should be "<Unset>."

2.2 How Are Algorithms Added to Links?

By default, all algorithms available in the library that describe mass transfer between two compartments are automatically added to a link between these compartments when the link is created (see Section 1.1). To include only particular algorithms on a link, the user can use a Property Import file to create the link and specify the algorithms on the link (see Figure 3 for an example of a Property Import file and Module 3 for additional details on specifying algorithms for a link in the Property Import file). Alternatively, the undesired algorithms can be removed from the link by selecting and deleting them. However, the current version of the TRIM.FaTE library does not contain multiple algorithms enabled for the same process. Users should be aware that if additional chemicals are added to a simulation after creating the links, the algorithms applicable to the newly added chemicals will not be included in the scenario. To avoid this problem, all chemicals should be added to the scenario prior to creating links. If chemicals are added later, links can be deleted (via select all and delete) and re-added.

2.3 Why and How Are Algorithms Removed from a Link?

For various purposes (e.g., evaluation or diagnostic purposes), the user may wish to perform a simulation without the transfer or transformation process described by a particular algorithm. To eliminate movement of mass via that particular algorithm, that algorithm can be either removed from one or more links specified by the user or disabled, depending on the particular objective. If the user disables an algorithm, that algorithm will be disabled on all links on which it appears in the scenario. The user should choose to either remove or disable an algorithm based on their particular goals, while carefully considering potential impacts.

To remove an algorithm from a link, the user should follow these steps.

- (1) Select a link (or links) associated with the algorithm in the Algorithms Tab. (See Figure 12 above)
- (2) Click the "Show Algs" button under the Outdoor Environment pane.
- (3) Select the algorithm in the "Algorithms in Links" pane.
- (4) Click the "Delete" button under the Outdoor Environment pane. This step removes the algorithm from only the selected link.

To disable an algorithm without deleting it from the entire scenario, the user should follow these steps.

- (1) Select a link associated with the algorithm in the Algorithms Tab. (See Figure 12 above)
- (2) Click the "Show Algs" button under the Outdoor Environment pane.
- (3) Select the algorithm in the "Algorithms in Links" pane.
- (4) Click the "Properties" button under the Outdoor Environment pane.
- (5) Change the value of the *enabled* property to "false" in the Property Editor. This step disables the algorithm from all links in the scenario, not only from the selected link. It is not possible to disable an algorithm for one link without disabling it for all links! Thus, to prevent chemical mass transfer or transformation via a particular algorithm across one particular link, the user should disable that link, not the algorithm on that link. See Section 1.4 for more information on disabling links.

3. REFERENCES

U.S. EPA. 2002. U.S. Environmental Protection Agency. TRIM.FaTE Technical Support Document Volume I: Description of Module. EPA 453/R-02-011a. Office of Air Quality Planning and Standards.

